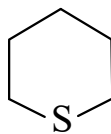




>>Entry Name: Tetrahydro-2H-thiopyran, 9CI

Synonym(s): Thian. Pentamethylene sulfide. Thiacyclohexane. Penthiophane



CAS Registry Number: 1613-51-0

Molecular Formula: C₅H₁₀S

Molecular Weight: 102.2

Accurate Mass: 102.05032

Percentage Composition: C 58.76%; H 9.86%; S 31.38%

Source/Synthesis: Found in petroleum

Physical Description: Cryst.

Melting Point: Mp 19.07°

Boiling Point: Bp 142°

Solubility: Insol. H₂O

Refractive Index: n_D²⁰ 1.5066

Other Data: Steam-volatile

Aldrich: P700-2

>>Derivative: Methiodide

CAS Registry Number: 72493-15-3

Physical Description: Needles (EtOH)

Solubility: Sol. H₂O; spar. sol. EtOH, insol; Et₂O, C₆H₆, petrol

Other Data: Subl. at 192° without melting

>>Derivative: S-Oxide

Synonym(s): Thian sulfoxide. Pentamethylene sulfoxide

CAS Registry Number: 4988-34-5

Molecular Formula: C₅H₁₀OS

Molecular Weight: 118.199

Accurate Mass: 118.045235

Percentage Composition: C 50.81%; H 8.53%; O 13.54%; S 27.13%

Melting Point: Mp 67-68°

>>Derivative: S,S-Dioxide

Synonym(s): Thian sulfone. Pentamethylene sulfone

CAS Registry Number: 4988-33-4

Molecular Formula: C₅H₁₀O₂S

Molecular Weight: 134.199

Accurate Mass: 134.04015

Percentage Composition: C 44.75%; H 7.51%; O 23.84%; S 23.89%

Physical Description: Cryst. (H₂O)

Melting Point: Mp 98.5-99°

Solubility: Sol. H₂O, EtOH; spar. sol. Et₂O, insol; petrol

Rare Chemicals Library: S77565-7

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 434B, (*nmr*)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 271B, (*ir*)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 356B, (*ir*)

v. Braun, J. *et al.*, *Ber.*, 1910, **43**, 545, (*synth*)

Clarke, H.T., *J.C.S.*, 1912, **101**, 1788, (*synth*)

Adv. Chem. Ser., 1955, **15**, 503, (*props*)

Lambert, J.B. *et al.*, *J.A.C.S.*, 1972, **94**, 8172, (*pmr*)

Org. Synth., Coll. Vol., 5, 1973, 791, (*oxide*)

Tezuka, T. *et al.*, *Tet. Lett.*, 1978, 1959, (*oxide*)

Nagasawa, K. *et al.*, *Chem. Pharm. Bull.*, 1982, **30**, 4189; 1985, **33**, 5048, (*synth, cmr*)

Satyamurthy, N. *et al.*, *Phosphorus Sulfur Relat. Elem.*, 1984, **19**, 113, (*cmr*)

Lowe, G. *et al.*, *J.A.C.S.*, 1988, **110**, 8512, (*dioxide, synth, cryst struct*)

Clennan, E.L. *et al.*, *J.A.C.S.*, 1992, **114**, 3021, (*oxides, synth, cmr*)